Glutaric acid, 2,2-dichloroethyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C13H12BrCl2FO4/c14-9-6-8(17)4-5-10(9)21-13(19)3-1-2-12(18)20-7-11(15)16/

InchiKey: XAWSXUUBKFACPK-UHFFFAOYSA-N

Formula: C13H12BrCl2FO4

SMILES: O=C(CCCC(=O)Oc1ccc(F)cc1Br)OCC(Cl)Cl

Mol. weight [g/mol]: 402.04

Physical Properties

Property code	Value	Unit	Source
gf	-522.90	kJ/mol	Joback Method
hf	-794.20	kJ/mol	Joback Method
hfus	41.50	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.011		Crippen Method
mcvol	228.900	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	2336.00		NIST Webbook
rinpol	2336.00		NIST Webbook
tb	825.91	K	Joback Method
tc	1047.34	K	Joback Method
tf	537.28	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.81	J/mol×K	825.91	Joback Method
cpg	584.67	J/mol×K	862.81	Joback Method
cpg	593.65	J/mol×K	899.72	Joback Method
cpg	601.75	J/mol×K	936.62	Joback Method
cpg	608.99	J/mol×K	973.53	Joback Method
cpg	615.39	J/mol×K	1010.43	Joback Method
cpg	620.95	J/mol×K	1047.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume